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CHEMICAL REACTING FLOWS

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This paper describes the objectives and accomplishments of research in chemical reacting flows, including both experimental and computational programs. The experimental research emphasizes the acquisition of reliable reacting-flow data for code validation, the development of chemical kinetics mechanisms, and the understanding of two-phase flow dynamics. Typical results from two nonreacting spray studies are presented. The computational fluid dynamics (CFD) research emphasizes the development of efficient and accurate algorithms and codes, as well as validation of methods and modelling (turbulence and kinetics) for reacting flows. Major developments of the RPLUS code and its application to mixing concepts, the General Electric combustor, and the Government baseline engine for the National Aerospace Plane are detailed. Finally, the turbulence research in the newly established Center for Modelling of Turbulence and Transition (CMOTT) is described.

Chemical Reacting Flows

Goal:

Development of accurate predictive CFD codes which simulate the coupling of fluid mechanics and chemistry of combustors of aerospace propulsion systems

- **Experimental research to investigate the physics and chemistry**
- **Provision of a proper data set for code validation and assessment**

Impact:

- **Ability to design aeropropulsion systems with performance at least double that of current engine technology**
- **Resolution of technical issues related to propulsion of hypersonic vehicles**

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The long-range goal of the Chemical Reacting Flows research program is the development and validation of predictive, time accurate, three-dimensional computational fluid dynamics (CFD) codes that simulate the coupling of fluid mechanics and combustion kinetics of combustors for aerospace propulsion systems. Drivers of the research activity are future requirements for major performance increases in hydrocarbon-fueled gas turbine engines that will operate at considerably higher pressures and temperatures than current engines, requirements for large reductions in emissions to minimize environmental impact of combustors designed for supersonic cruise, and a need to gain a better understanding of combustion chemistry and mixing interactions for hydrogen-fueled combustion systems of hypersonic vehicles.

The major activities of the program, in addition to the development of reliable time-accurate codes, are fundamental experimental and analytical research on combustion kinetics, experimental study of the interactions of fluid dynamics and chemistry, and the development of detailed reacting-flow datasets for code validation and assessment.

Hydrocarbon Combustion

- Advanced methods for reacting flow calculations
  - Numerical methods and physical models for combustion of liquid fuel sprays in a high-pressure, high-temperature environment
- Two-phase flow modeling and experiments
- Hydrocarbon kinetic mechanism development
- Chemical kinetics mechanism reduction
  - Efficient utilization of reacting-flow Navier-Stokes codes

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The research in hydrocarbon combustion can be divided into three areas:

(1) Development of a fast, robust, three-dimensional Navier-Stokes code for low-speed reacting flow - including an improved physical model of the evaporation and combustion of hydrocarbon fuel sprays, advanced turbulence and mixing models, and reduced hydrocarbon kinetic mechanisms that reduce computational overhead yet adequately reproduce heat release and combustion emissions

(2) An experimental and modelling program for combusting hydrocarbon sprays to obtain detailed measurements and understanding of the physical processes of two-phase flow for development and assessment of the CFD codes

(3) Experimental measurements and modelling of hydrocarbon kinetics and mechanisms with emphasis on predicting formation of nitrogen oxides and soot (Reduced mechanisms will be developed and compared with more complete mechanisms by using flame codes and experiments.)

The research program for two-phase flow of liquid fuel sprays in air will now be shown in more detail.

Two–Phase Flow Modeling and Experiments

Objective:

- **Perform experiments to increase understanding of physics of multiphase flows and obtain data base for validation of multiphase flow codes**

Approach:

- **Perform series of experiments with increasing complexity**

  - **Particle-laden swirling flows**
  - **Nonreacting sprays**
  - **Unconfined combusting sprays**
  - **Confined combusting sprays**
  - **Pressurized combusting sprays**

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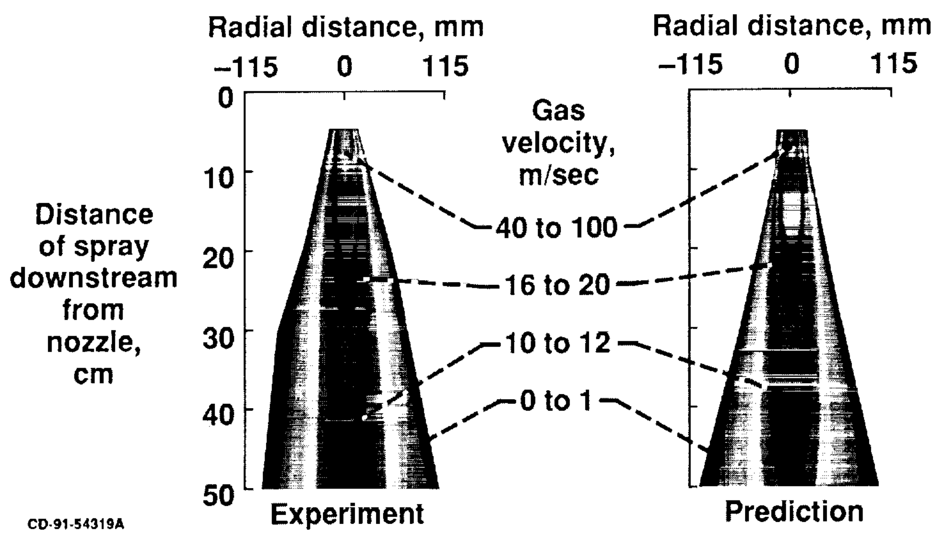
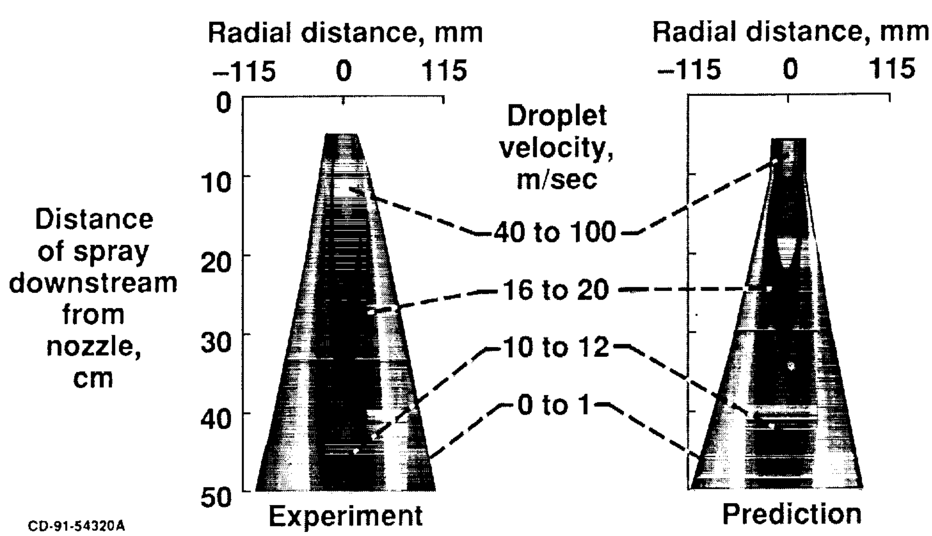
The fuel-spray process is extremely important for engine efficiency, durability, and operability. The ultimate objective of this research is to develop a computer code that can accurately model fuel and air mixing with the subsequent reaction. Since this is an extremely complicated process, we are studying it in a series of steps of increasing complexity. Particle-laden jets were initially studied followed by non-reacting sprays to assess the capability of current two-phase flow models. Typical results from the nonreacting spray study are illustrated in the following figures. Currently, unconfined combusting spray experiments are being conducted and will be used to assess the capability of reacting, multiphase flow codes. Future plans are to study confined atmospheric, and then, pressurized combusting, sprays.

Axial Gas Velocity for Nonreacting Spray

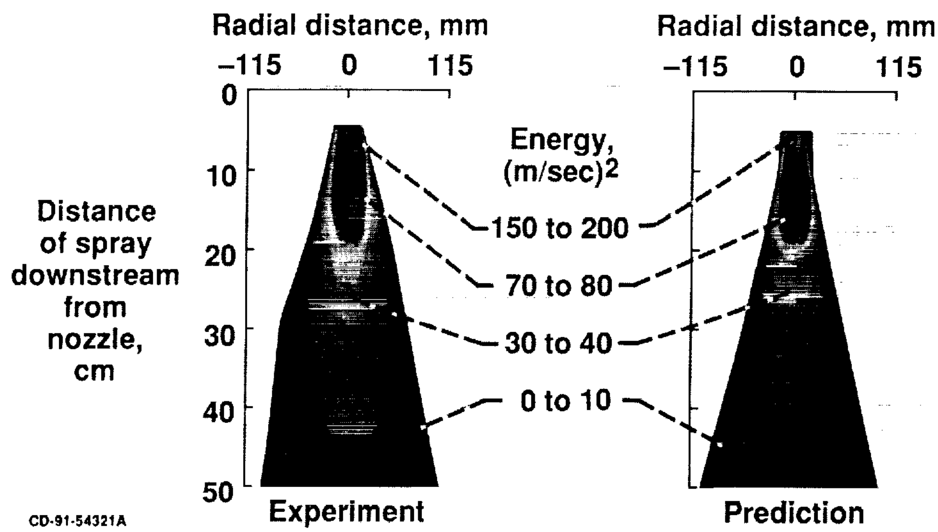


Mean Axial Droplet Velocity (25 μm) for Nonreacting Spray



These figures compare measured and predicted axial velocities for the nonreacting spray. The experiment consisted of an air-assist atomizer spraying vertically downward into a stagnant environment. Mean axial velocities for the gas phase and 18-μm droplets are illustrated for the spray from 5- to 50-cm downstream of the nozzle. Velocity measurements were made with a two-component Phase/Doppler particle analyzer and were obtained across the entire spray. Contour levels are illustrated for velocities from 0 to 100 m/sec, and radial dimensions are in millimeters. It is evident that the spray was very axisymmetric, making it useful for model comparison. The computer model utilized for the predictions is a parabolic model with Lagrangian tracking of the particles in the computed gas-phase flowfield. Source terms are included to account for momentum exchange between the droplets and the gas phase. Turbulent dispersion of the droplets is also considered. Predictions show reasonable agreement with the data for the decay of both gas phase and droplet velocity.

Turbulent Kinetic Energy



This figure compares measured and predicted gas-phase turbulent kinetic energy in the spray flowfield. Predictions were obtained with the k-ϵ turbulence model. Contour levels are illustrated from 0 to 200 $(m/sec)^2$ for the spray flowfield from 5- to 50-cm downstream of the nozzle. Radial dimensions are in millimeters. Again, the agreement between the predictions and measurements is reasonably good.

Unconfined Combusting Spray

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This photograph shows the unconfined combusting spray. The experiment consists of an air-assist atomizer spraying n-heptane liquid fuel upward into a coflowing swirling air stream. This coflow stream was swirled sufficiently by a 45° swirler to generate a recirculation zone that stabilized the flame. A thin light sheet from a copper vapor laser was used to illuminate the trajectories of the liquid fuel droplets in the combusting spray. Experimental measurements will include gas phase and droplet velocities, gas phase temperatures, and major species.

Hydrogen Combustion

Requirement:

- **Understanding of the interaction of fluid dynamics and chemistry in high-speed propulsion devices which have high subsonic and/or supersonic combustors**

Enabling technology:

- **Development of both steady and unsteady Navier-Stokes codes for analyses of combustion systems with emphasis on increased computational efficiency and improved modeling of physical processes**
- **Data sets for high-speed reacting shear layers**
- **Improved chemical model for the hydrogen-air system**

Goal:

Ability to design efficient combustion systems and accurately predict combustor performance for future hypersonic vehicles

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The research in hydrogen combustion is directed toward applications to high subsonic or supersonic combustion in propulsion systems for hypersonic vehicles. Emphasis of the research program is the development and assessment of three-dimensional, reacting-flow Navier-Stokes codes which will be covered subsequently: experimental research on high-speed turbulent reacting flows to (1) improve the understanding of coupling between fluid dynamics and combustion, and (2) establish a dataset to validate computer codes which simulate the physics and chemistry of high-speed chemical reacting flows. Experimental and analytical studies of hydrogen-air kinetic rates and modelling are also being conducted which are relevant to ignition, kinetics losses, and ground test facility simulation issues for supersonic combustion.

Hydrogen Combustion–
Program Elements

- **Planar reacting shear layer**
  - **Experimental database for CFD code validation**
  - **Understanding of turbulence-chemistry interactions**
- **Hydrogen-air kinetics rates and mechanism development**
- **Computational studies of the Ram-Accelerator**
  - **Propulsion and test facility applications**

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Research in hydrogen combustion is directed in three areas:

(1) A planar reacting shear layer experiment is being studied to obtain steady-state reacting hydrogen data of mean and fluctuating velocities and concentrations, to compare benchmark data with predictions from computer models, and to evaluate turbulence-chemistry interactions. The experiment is designed to mix and react two streams downstream of a splitter plate. One of the streams is hydrogen that is diluted with nitrogen and the other is air that is preheated up to 870 K. Flow rates are continuous at high subsonic velocities. The facility is now operational, and Mie scattering data are being obtained for initially nonreacting streams.

(2) Reaction rates for hydrogen-air are being obtained in a chemical shock tube that uses laser absorption diagnostics to measure hydroxyl radical concentrations. The objective is the determination of three-body recombination rates of hydrogen and oxygen and the effect of water on these rates. Radical and atom recombination rates are particularly important in determining kinetic losses in exhaust nozzles of hypersonic vehicles.

(3) A computational program is in progress on the Ram-Accelerator concept to supplement experimental work at the University of Washington. In this concept, the centerbody of a shaped projectile is fired into a tube containing premixed fuel and oxidizer. Combustion occurs in either a subsonic, supersonic, or stabilized detonation mode between the projectile and the tube, creating a high-pressure region behind the projectile to accelerate the projectile to hypersonic velocities. The computational analysis is carried out with the fully coupled, Reynolds-averaged Navier-Stokes equations. Results include shock-boundary interactions and forebody precombustion effects that give credence to the process.

Chemical Reacting Flows—CFD Goals

- Develop reliable, versatile, 3-D CFD codes for chemical reacting flows for practical geometries and conditions
- Support national programs and industry needs

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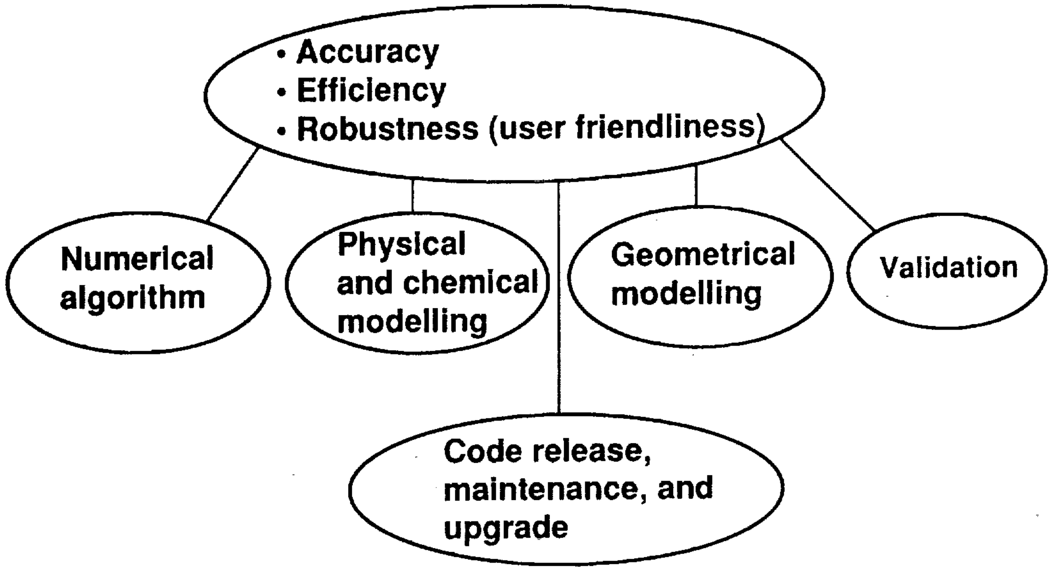
Our CFD goals for chemical reacting flows are shown above. Here at NASA Lewis Research Center, we are responsible for developing three-dimensional CFD codes that are reliable in accuracy and are versatile - able to accept complex geometries and flow conditions. The codes are designed to efficiently solve equations describing viscous, finite-rate chemical reacting flows. Another objective is to closely support national programs and industry needs in aeropropulsion systems, such as the National Aerospace Plane (NASP) and the High-Speed Civil Transport (HSCT). In order to accomplish these goals, a substantial emphasis is placed on the following issues related to CFD.

Issues of CFD



This chart describes the essential requirements that a CFD code must take into consideration: namely accuracy, efficiency, and robustness (or user friendliness). Whether or not these requirements can be successfully met critically depends on the following building blocks: (1) the numerical algorithm, (2) the physical and chemical models, (3) the geometrical model, and (4) validation. All of these have been under intensive research and development in the past 20 years and are still evolving to meet the three requirements.

Here at Lewis, we are studying every aspect of these building blocks. For the numerical algorithm, we have developed a unique, efficient algorithm which is especially suited for solving a large system of equations in chemical reacting flows. The resulting code is called RPLUS and its various versions have been released to many institutions in the country. This paper describes three studies carried out at Lewis and General Electric (the latter, a case of close collaboration between Lewis and industry). We are also looking at some forefront numerical methods to improve accuracy and efficiency. In physical and chemical modelling, and especially in turbulence modelling, a strong and focused group, the Center for Modelling Turbulence and Transition (CMOTT), has been at the Institute for Computational Mechanics in Propulsion (ICOMP) at Lewis for over a year. This group has been taking rigorous approaches, ranging from accessing effects of numerical dissipations to developing new models for treating effects like compressibility and turbulence/chemical interactions. In geometrical modelling, we are looking at surface- and field-grids generation, as well as multiblocking and adaptation in the CFD codes. Finally, the ultimate test is the validation of the code. This never-ending process requires a more in-depth comparison as measurements provide more information and as physical models become more sophisticated. The research and development in CFD are ever-evolving, and these requirements will only become more stringent. Our CFD goal, ultimately, is to release and maintain codes developed at Lewis. The codes will be continually upgraded as building blocks are improved. In the rest of this paper, I will discuss the progress in these areas.

Development of RPLUS Code

- Development under the NASP TMP (1988 to 1990), and support continued under generic hypersonic program
- Code released to U.S. industry, universities, and government labs (over 40 releases)
- The code currently has the following capabilities:
  - 3-D, Navier-Stokes equations with finite-rate chemical reactions
  - Multiblock decomposition for geometrical flexibility
  - Baldwin-Lomax and k-ε models
  - Central and upwind differencing

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The development of the RPLUS code was originally funded under the NASP Technical Maturation Plan (TMP) which began in 1988 and ended in 1990. Starting in 1991, the funding was picked up under NASA's generic hypersonic program. Various versions of the code have been released to requesters from U.S. industry, academia, and government labs, totaling over 40 copies. One workshop was held in the fall of 1988. We have designated contact persons for handling the transmission as well as for answering questions regarding the code. Several requesters have spent time at Lewis becoming familiar with the intricate details of the code and the theory. We have also incorporated some valuable input from the users. Such two-way dialogues were found to have great mutual benefits.

The code solves three-dimensional, Navier-Stokes equations coupled with finite-rate chemical kinetics equations. In the case of H_2-air reactions, 9 species and 18 reaction steps were considered, resulting in 13 conservation equations, rather than 5, to be solved. The chemical kinetics models are user-supplied and not hard-wired as an integral part of the code, thus giving flexibility. For complex geometries, it is difficult to generate a single grid without introducing distortion, which usually, in turn, reduces accuracy and stability. To avoid distortion, we adopt a multiblock approach - decomposing the entire domain into several blocks for which it is easy to generate a good quality grid. The global conservation is enforced in the treatment of interfaces. In addition to the Baldwin-Lomax model, the code includes several variations of the κ-ϵ model. An upwind version of the code is also available.

Representative Applications of RPLUS Codes

- Swept and unswept fuel injectors
- Government baseline engine
- General Electric combustor

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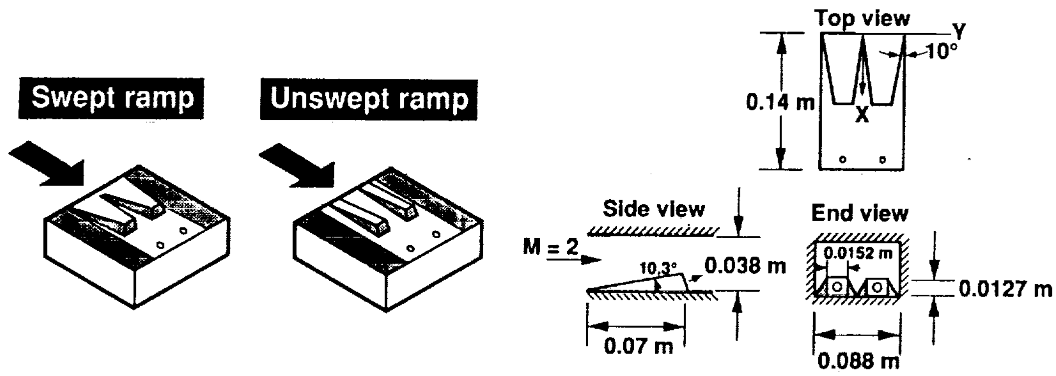
Next, we present some representative applications of the RPLUS code to demonstrate its capability and to ultimately shed some light on the fluid dynamic processes of design concepts. The calculations for the first two cases were carried out at Lewis by Young-June Moon and Beverly Duncan, respectively. The third case was performed by Mani Subramanian of GE and his group, in close collaboration with Peter Tsai and Tawit Chitsonboom. This case especially illustrates how much one can achieve by using a nondesign code to give design parameters.

Swept and Unswept Fuel Injectors



Incoming Stream

Mach number	2
Pressure, Pa	102 000
Temperature, K	1024
Mass fraction	
H_2O	0.182
O_2	0.256
N_2	0.562

Hydrogen Jet

Mach number	1.7
Pressure, Pa	325 200
Temperature, K	187
Equivalence ratio	1.2

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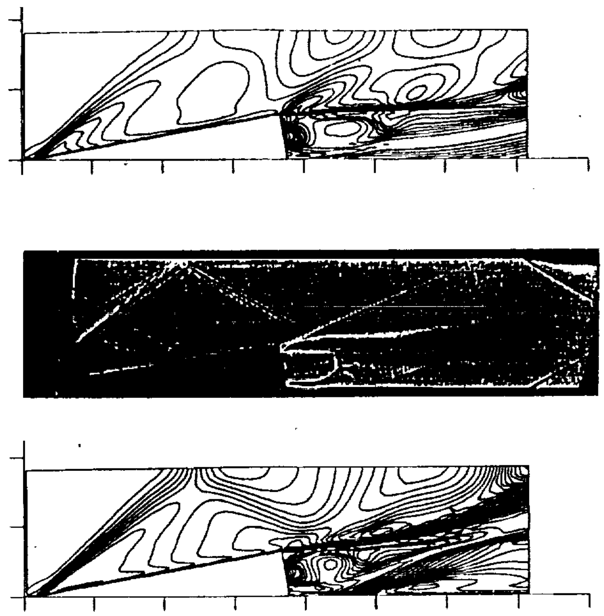
This figure shows the configuration of the fuel injectors for a supersonic combustor investigated experimentally by Northam et al. of NASA Langley Research Center. Since mixing is a crucial step for initiating chemical reactions and the mixing is diminished in high-speed streams, this configuration is used to study concepts to enhance mixing via generating streamwise vorticity. The flow conditions are given above.

Because of the ramp and corner topologies and the requirement of the fine grid at the surfaces, a single grid gives rise to undesirable distortion and nearly singularities at the corners. These deformations generally lead to nonconvergence and excessive numerical dissipation. A multiblock strategy was used to overcome this difficulty, and as a result, the calculation became easy to handle. The grid densities are 0.16 and 0.17 million, respectively, for unswept and swept cases, each using three blocks.

Swept and Unswept Fuel Injectors (continued)

Density Contours



Unswept

Swept

Swept

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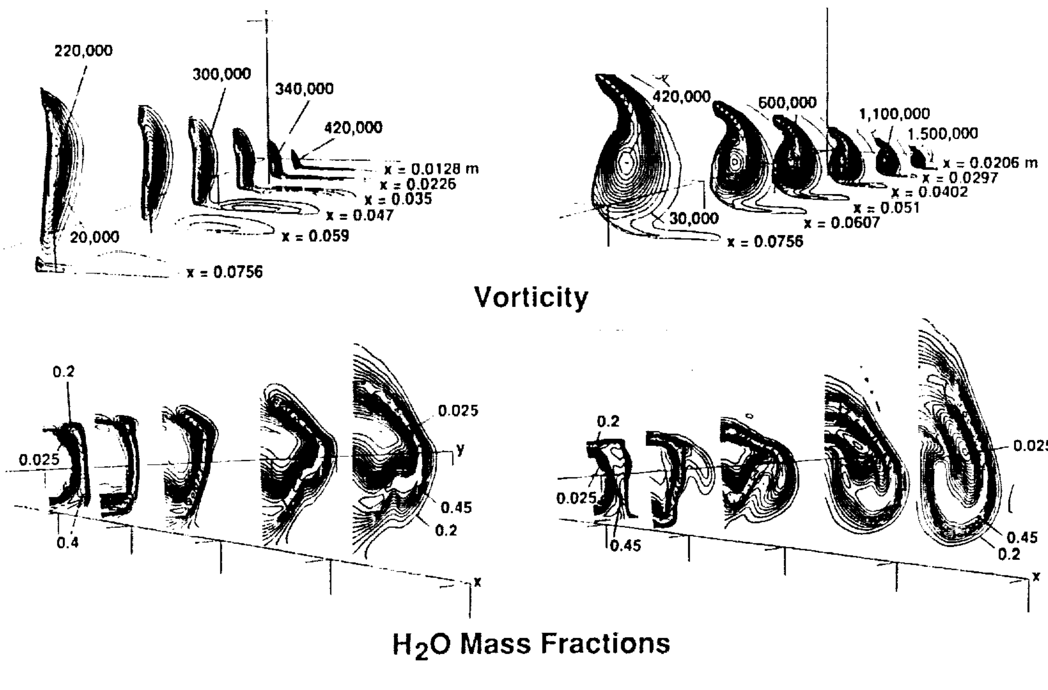
Here we show the density contours of both swept and unswept configurations at the jet centerplane and the comparison with the shadowgraph for the swept case. Qualitative features such as the shocks, expansion wave, fuel jet plume, and shear layer are well represented, despite the relatively coarse meshes utilized. Simply because of the difference in geometry, two effects are noticeable. In the swept case, because the leading edge is two dimensional, the ramp shock is stronger, and the subsequent reflected shock from the top wall remains stronger. Second, the fuel jet is lifted away from the ground more because of the induced motion by the stronger vorticity generated along the ramp edge.

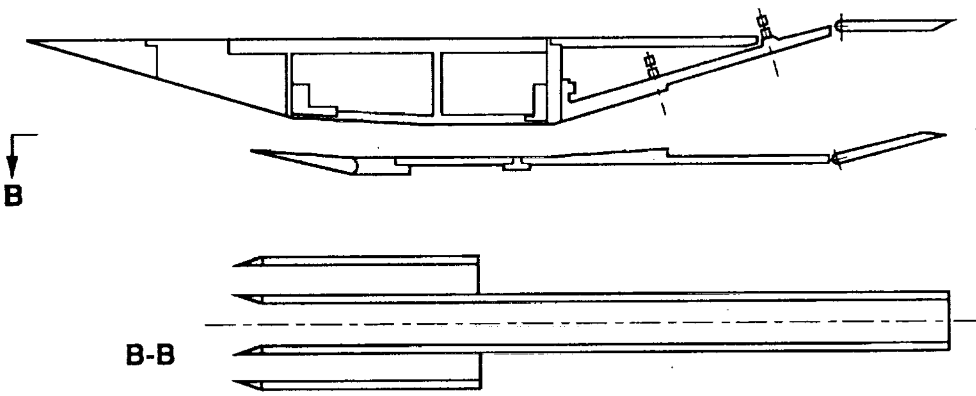
Swept and Unswept Fuel Injectors (concluded)

Vorticity and H_2O Contours



The vortical structure generated by the spanwise nonuniformity is clearly displayed at five cross planes upstream of the injector face. In the swept case, this vortical structure has much greater strength and grows in three dimensions, while in the unswept case, the spanwise growth is rather confined close to the ramp side wall. The water vapor concentrations are compared at five planes downstream of the injector. The fuel jet is seen more rapidly deformed and its core is merged quickly into the core of the vortex generated upstream at the ramp. Finally the core moves away spanwise from the jet centerplane, while the core of the unswept case is deformed but still remains at the centerplane. Thus, it is important that this vortical structure be generated and that its major growth take place sufficiently ahead of the injection so that the mixing of the two streams can be effective. This clearly shows the advantages of using the swept injector for promoting mixing and, thus, combustion.

Government Baseline Engine



Free-Stream Air	
Mach number	3.44
Total temperature, K	750
Total pressure, atm	4.2

Hydrogen Jet	
Mach number	1.0
Temperature, K	293
Equivalence ratio	0.4

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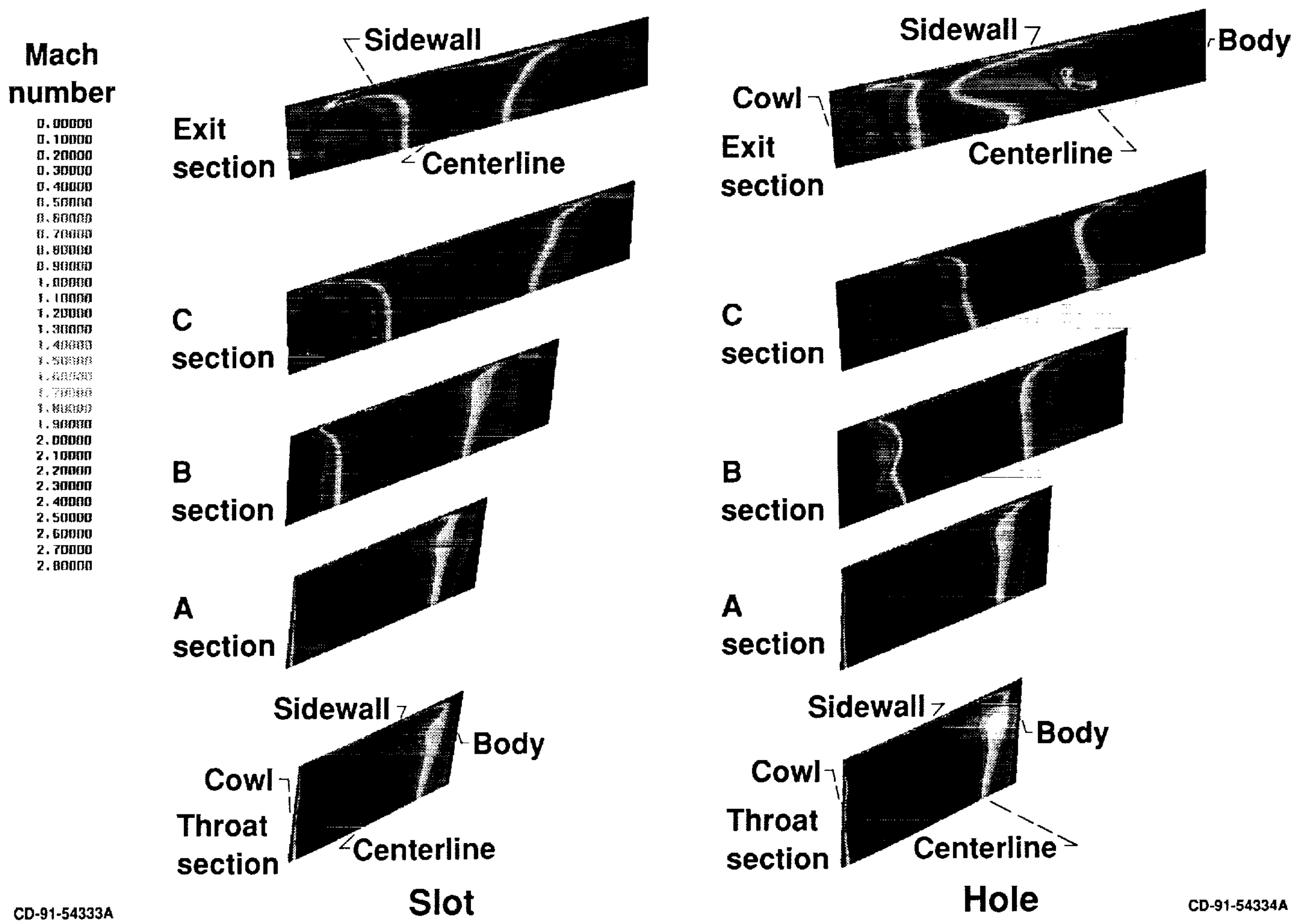
This sketch shows the Government baseline engine model used to study hypersonic propulsion concepts. The experiment was planned and carried out by Dave Sagerser of Lewis. Then, the test was performed initially at General Applied Science Laboratories (GASL) and subsequently at Lewis. There is a synergistic coordination between the experimental and computational groups. An objective of the computational effort is to demonstrate the current CFD capability for calculating a complete "nose-to-tail" configuration, using a complicated set of chemical kinetics. We also studied the effects of slot and discrete fuel injectors on mixing and combustion, and valuable information can be extracted for examining new concepts. This case shows how CFD has become an indispensable and cost-effective tool in various phases of a design cycle, despite uncertainties regarding the previously mentioned building blocks, such as modelling and validation. The flow conditions are listed above, and laminar flow is assumed. The total mass of injection was kept the same to compare the effectiveness of the two injections; thus different injection pressures were required.

Government Baseline Engine (continued)

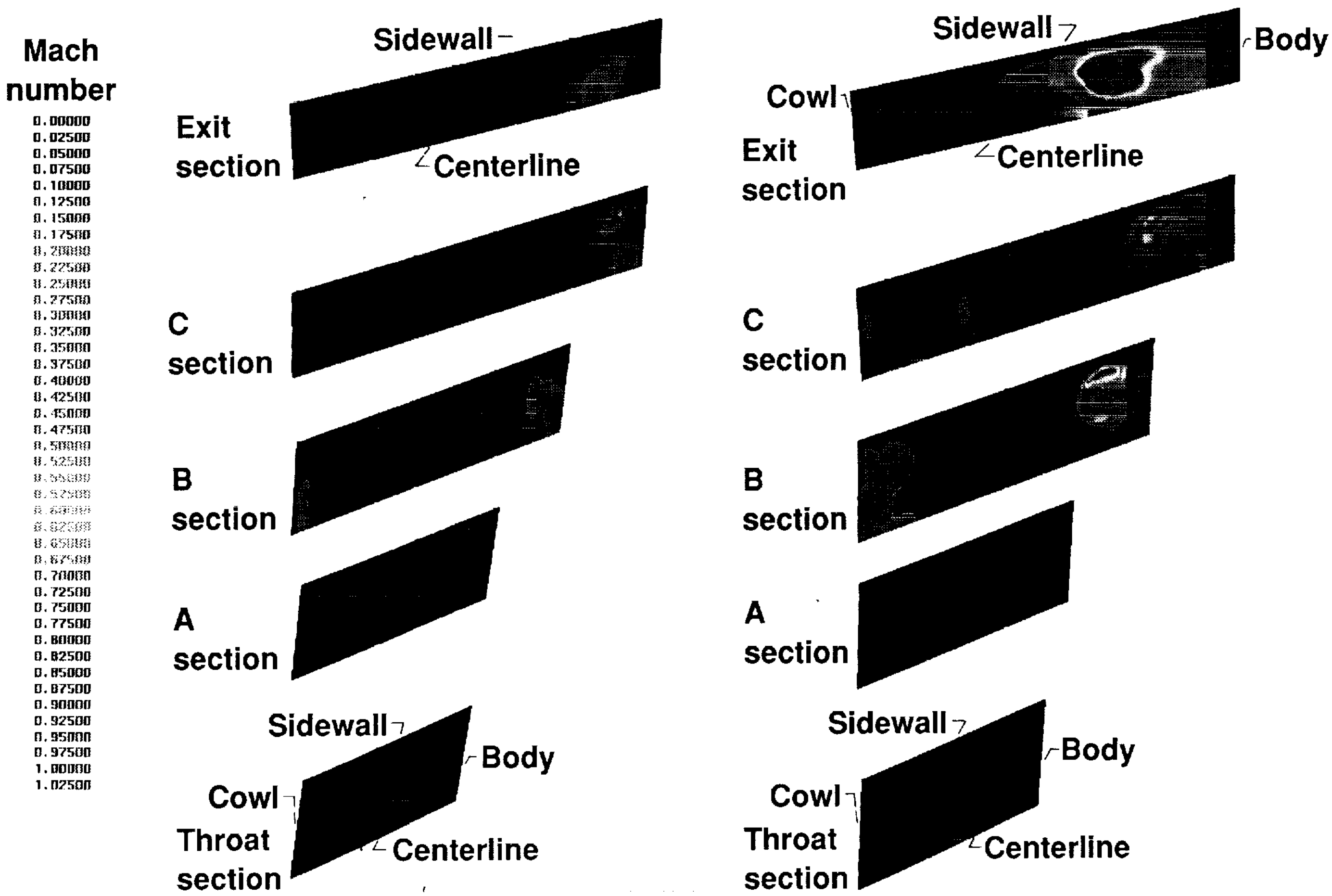
Mach Number Contours



This chart displays the Mach contours with the slot and discrete hole fuel injections in the engine. Five transverse planes, four located downstream of the injection port and one at the throat, were plotted to indicate the extent of mixing due to these two injections. The inviscid core and the low-momentum region near the walls are clearly visible. It is clear that the discrete injector provides much greater mixing since it generates a spanwise gradient. Thus streamwise vorticity is generated, and it, in turn, induces cross-plane velocity components which are responsible for enhancing the mixing. It is noted that the body side has better mixing than the cowl side. This is attributable to the thicker boundary layer initiated by the cowl shock and convected downstream. In the case of hole injection, a kidney-shaped secondary flow containing high vorticity is evident, and the nonuniformity at subsequent planes becomes increasingly stronger, leaving a greatly reduced inviscid core at the exit.

Government Baseline Engine (concluded)

H_2O Contours



CD-91-54335A Slot

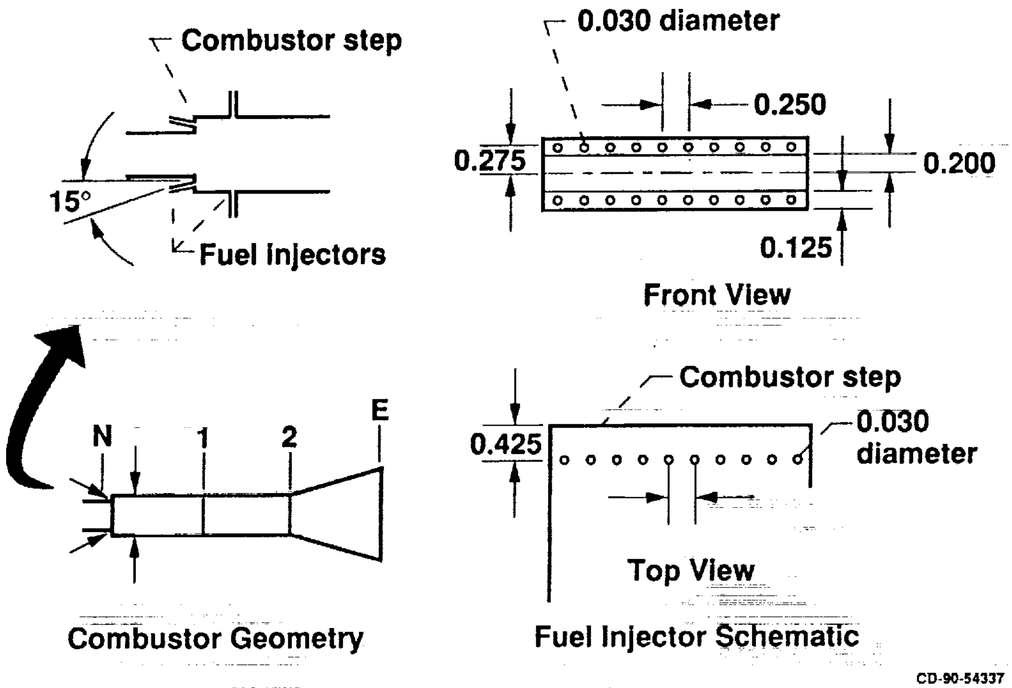
Hole CD-91-54336A

Here we show the extent of reaction due to the two injections. As expected, the higher the mixing, the better the combustion. A dramatic difference in the H_2O concentration clearly indicates the effectiveness of the hole injection, while the slot injection only allows the reaction to take place in limited regions. In both cases, since the air entering the combustor (even at adiabatic temperature) is at too low a temperature to ignite, a "torch ignitor" is placed in the computation.

The computational results will give extremely useful guidelines to researchers planning experiments, particularly in such complicated fluid dynamic situations where little information is known a priori. The experimental data are being generated and processed. Detailed comparison will follow and should clarify the areas that need further investigation. Currently both efforts of test and computation are continuing.

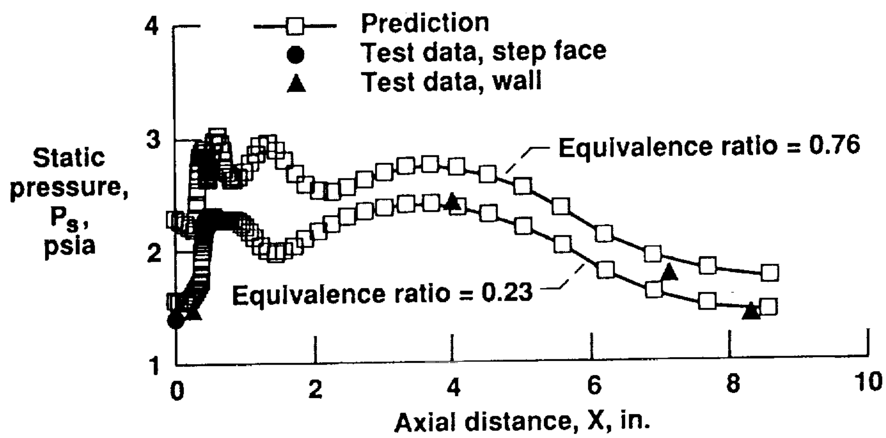
General Electric Combustor

- Dimensions are in inches



This figure shows the geometry of the GE scramjet combustor which was measured at the Ohio State University. A very extensive interrogation of the RPLUS code was performed by the GE group led by Subramanian. A detailed study of flow physics and mixing in this combustor was conducted for Mach numbers from 3 to 6. A number of injection geometries and arrangements were investigated. The flow conditions are shown in the figure. The Baldwin-Lomax model was extended to account for three-dimensional corner effects. The heat releases of various configurations were compared, and an extensive set of design parameters were examined to assess the performance. Also shown are the geometries of the injectors, including the circular hole and the normal and slanted slit-slot.

General Electric Combustor (continued)
Particle Traces and Wall Pressure



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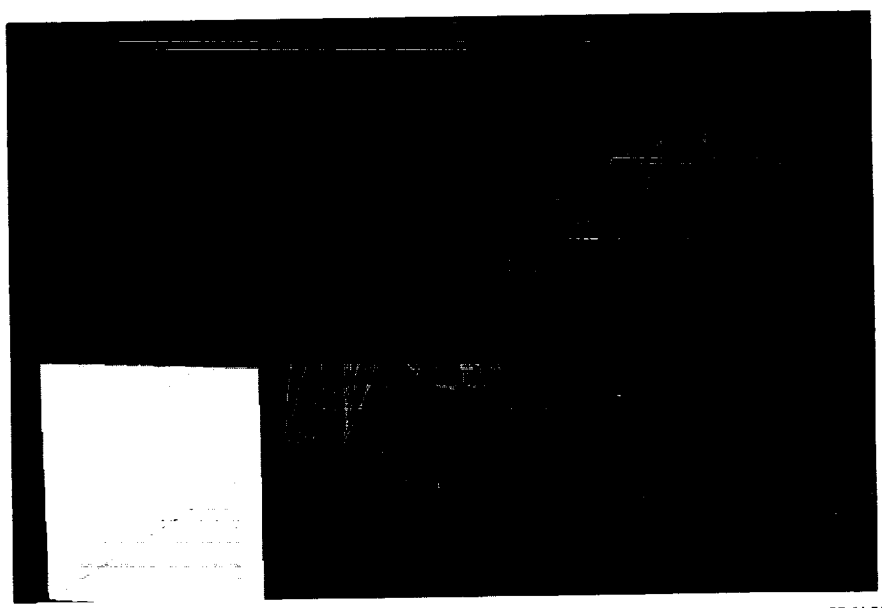
Scramjet Combustor Geometry
Particle Traces
[Equivalence ratio = 0.76]



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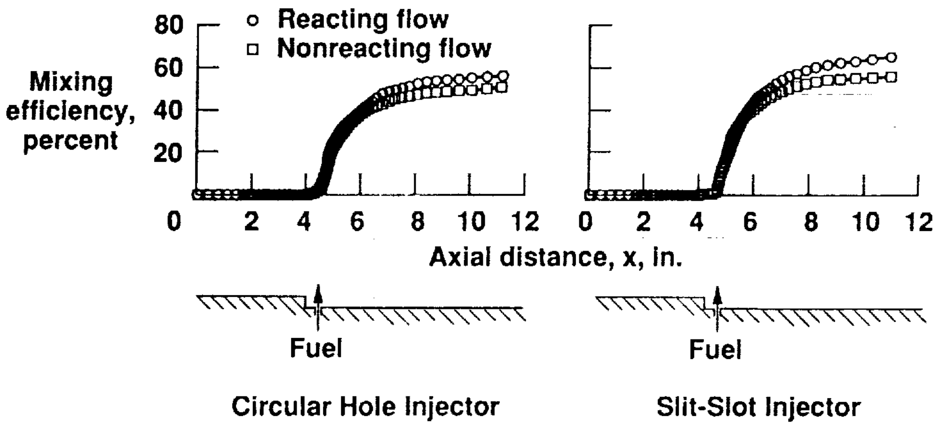
Shown in this chart are the three-dimensional view of particle traces and the pressure distribution along the bottom wall at midway between normal jets. The test was performed at the Ohio State University with an upstream Mach 3 condition. Few data points that are available appear in good agreement with the calculations. The particle traces also clearly show the vortical structure and the entrainment of free stream fluid into a spiral motion. However, at about twice the step-height the stream does not mix with the injected hydrogen anywhere in the combustor. Next, various injection concepts are examined to assess their performance.

General Electric Combustor (concluded)
Injector Geometries and Mixing Efficiency

[Equivalence ratio = 1.5, Mach number = 18, dynamic pressure ratio = 2.0]



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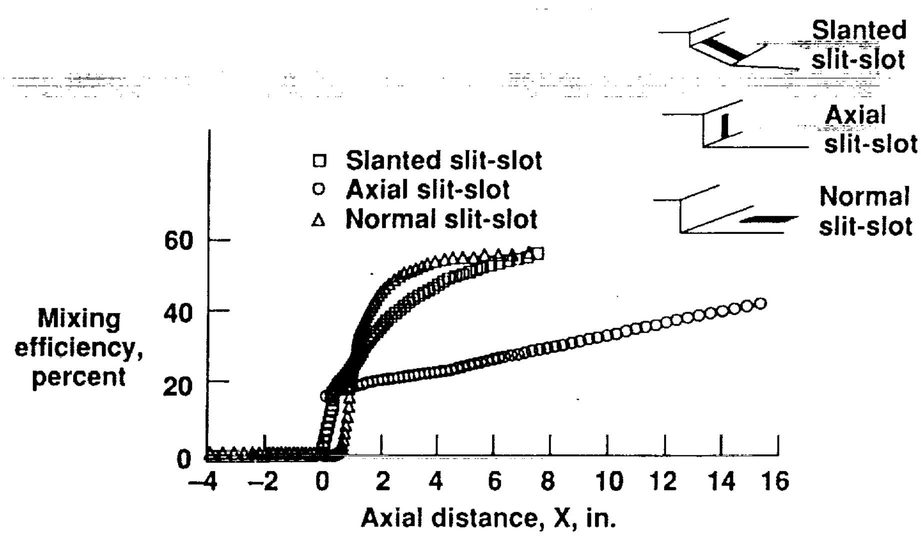
Mixing Efficiency Versus Axial Combustor Length

[Equivalence ratio = 1.5, Mach number = 18, dynamic pressure ratio = 2.0]



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On this page we compare mixing efficiencies of several injector configurations as well as the effect of the chemical reaction. The incoming conditions corresponding to a Mach 18 flight are $M = 6.7$, $P = 7.05$ psia, and $T = 3246$ °R. The fuel injector has conditions at $M = 2$, $P = 126$ psia, and $T = 1123$ °R. First the slit-slot injector appears to be about 5 to 10 percent more efficient than the circular injector, and the H_2-air chemical reaction actually promotes mixing. Thus, we focus now on varying the locations of the injector - at the bottom wall, the step face, or the slanted face. The bottom wall (normal) injection is the most efficient, and the axial injection at the step face is the least efficient. The collaborative effort between GE and Lewis is continuing, and the CFD information will continue to assist design modifications and performance improvements studies.

Turbulence Modelling

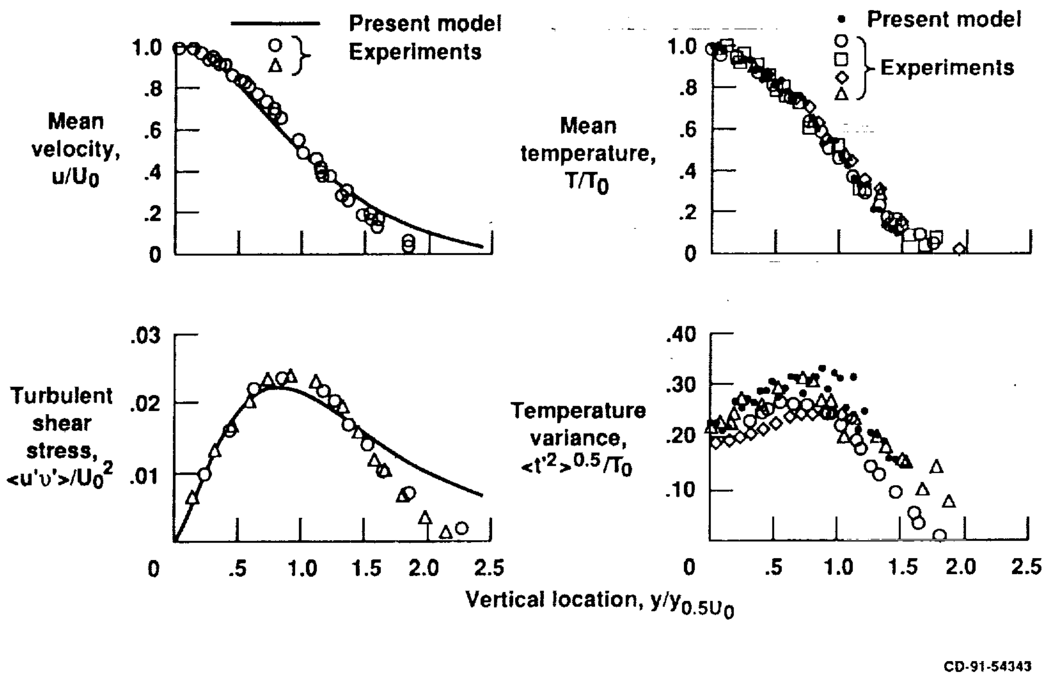
- **PDF turbulence combustion modelling**
- **Development of k-ε and second-moment models**

CD-91-54342

As I mentioned earlier, there has been considerable progress in turbulence modelling made by the CMOTT members at Lewis. We have been looking at using the probability density function (pdf) approach to represent the turbulence fluctuations due to chemical reactions. In the past year, significant effort has been spent on assessing the currently available two-equation models and second-order models. In the next two pages, I present only two of these cases to show some of the significant results.

PDF Turbulence Modeling

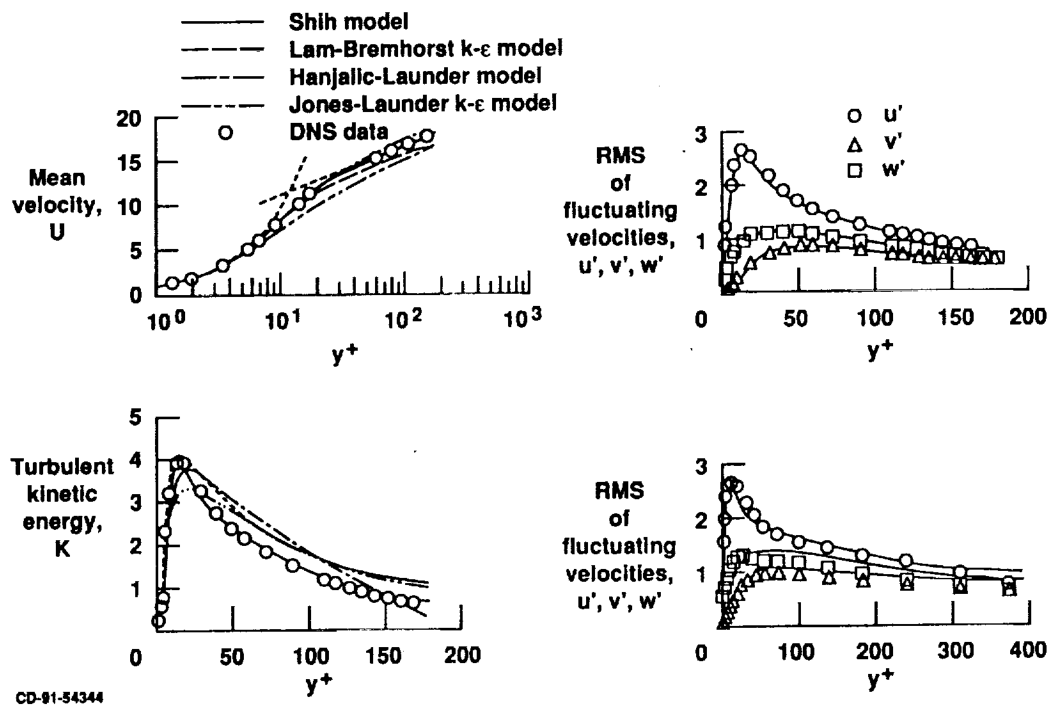
Heated Turbulent Free Jet



This figure shows calculated solutions of a heated turbulent free jet using a pdf model by Andrew Hsu. Good agreement of mean velocity and temperature distributions with experimental data is obtained. The correlations of fluctuating quantities are also included for comparison. Except a slight over-prediction near the edge of the jet, the numerical Reynolds shear stress generally agrees well with the data. An accurate prediction of the Reynolds stress terms is essential for the correct modelling of molecular mixing in the pdf calculation. Also, the calculated temperature standard variance agrees very well with the experimental observations. An accurate representation of temperature fluctuations is particularly important in chemical reactions because the reaction rate is strongly dependent on the instantaneous temperature.

Second-Moment Turbulence Modelling

Channel Flow



This page shows the results of using higher-order turbulence models for channel flow. T.-H. Shih, who serves as the technical leader of CMOTT, has been developing second-moment closure and κ-ϵ models. Although theoretical justification has been employed to the maximum extent possible in the development of turbulence models, experimental observation and measurement have also been indispensable. With the rapid growth of computer power, there is a new source of information: the direct numerical simulation of the Navier-Stokes equation is now possible, but it is limited to low Reynolds numbers. This figure compares results from two κ-ϵ models and two second-moment models with the direct numerical simulation (DNS) data. Shih's model, which is indicated by the solid line, has produced both mean and fluctuating results in excellent agreement with the DNS data, in particular the peaks show excellent agreement. Further efforts in compressible turbulence model development and verification for more complex flows for the second-moment closures are well underway.

Current and Future Research

- Development of advanced numerical algorithms
- Development of compressible k-ε and second-moment models
- Incorporation of interactive (menu-driven) grid generation in the RPLUS code
- Continuing validation of the code and models
- Continuing support of onsite and offsite research and development

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This chart summarizes some of the current and future research in terms of the four building blocks described earlier: namely, in the areas of developing advanced numerical algorithms, physical and geometrical models, and validations. Research on new algorithms has resulted in several promising possibilities. Also, significant collaboration with ICOMP researchers has been maintained. Now, compressible models are being developed by taking the direct interaction (DIA), renormalization group (RNG), and second-moment approaches. Research on using menu-driven ideas for interactively generating grids has been conducted in the last few years, and Yung Choo and Peter Eiseman plan to implement this research into the RPLUS code. As stated over and over again, the validation of the RPLUS code and models is continuing by examining more complex flows and more complete and reliable data sets. Last, but not least, we fully believe in supporting relevant onsite and offsite programs and welcome the opportunity of participation.